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Ab initio study of a class of metalorganic systems HARALD O. JESCHKE, L. ANDREA SALGUERO, ROSER VALENTI, Institut für theoretische Physik, Johann Wolfgang Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt/Main, Germany, BADIUR RAHAMAN, TANUSRI SAHA-DASGUPTA, S.N.Bose National Centre for Basic Sciences, J.D Block, Sector 3, Salt Lake City, Kolkata 700098, India, CHRISTIAN BUCHSBAUM, MARTIN U. SCHMIDT, MATTHIAS WAGNER, Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe-Universität, Marie Curie-Str. 11, 60439 Frankfurt/Main, Germany — We use first principles methods to study the electronic properties of a Cu(II) coordination polymer. We have introduced two substitutions on the polymer in order to investigate the influence of the change of constituents in the hydroquinone molecule on the interactions between the metal centers. Furthermore, we have introduced two different ligand molecules in order to simulate the effect of satellite molecules in a real sample in the laboratory. In the preparation and analysis of the structures, we optimize computational efficiency and precision by employing four different methods: We initially prepare structures with classical force field methods, then we relax the rough structure by ab initio molecular dynamics. The analysis is done with a full-potential linearized augmented plane-wave (LAPW) method and by downfolding with the N-th order muffin tin orbitals (NMTO) method. We find subtle changes of the interaction between the metal centers and of the band structure with each substituent or ligand molecule.

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